WEAK HYDROGEN BONDING IN COMPLEXES OF SELENOPHENE AND WATER: A MATRIX ISOLATION FTIR AND COMPUTATIONAL STUDY

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Weakly-bound complexes containing aromatic species have been the subject of study for many years. Here, a study of the weakly-bound complexes of selenophene (C_4H_4Se) with water will be presented. In this study, matrix isolation FTIR and computational methods were used to examine stable 1:1 complexes of selenophene : water (Sp:H_2O). Multiple density functional theories along with MP2 calculations were used to find a total of seven stable geometries which could be sorted into four categories defined by the intermolecular forces observed in the complex. The interactions include O$-$H$\cdots$Se, O$-$H$\cdots\pi$, and C$-$H$\cdots$O. The Sp:H_2O geometries were found to be within 16 kJ/mol of each other across all computational methods. All calculated structures were similar to those found for complexes of furan : water and thiophene: water. Matrix isolation FTIR experiments identified several peaks that were not associated with isolated water or selenophene, implying the bands are due to weakly-bound complexes of the two monomers. In addition to normal water, D_2O and HDO complexes with selenophene were also observed. Possible interpretations of the experimental and computational results will be presented.